(FILE 'HOME' ENTERED AT 15:10:45 ON 11 MAY 2004)

FILE 'REGISTRY' ENTERED AT 15:11:01 ON 11 MAY 2004

L1 STRUCTURE UPLOADED

12 S L1 ь2

214 S L1 SSS FULL L3

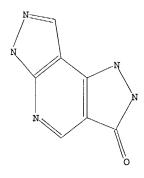
FILE 'CAPLUS' ENTERED AT 15:12:10 ON 11 MAY 2004

10 S L3 L4

=> d 11

L1 HAS NO ANSWERS

L1



Structure attributes must be viewed using STN Express query preparation.

=> d 1-10 bib abs hitstr

ANSWER 1 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN L4

2004:182530 CAPLUS AN

DN140:235704

Preparation of dihydrodipyrazolopyridinones as B7-1/CD28 binding inhibitors for the immunotherapeutic treatment of organ transplant rejection

Green, Neal Jeffrey; Tam, Steve Yikkai; Xiang, Jason Shaoyun; Davies, Audrey Molina; Chen, Lihren; Stack, Gary Paul IN

Air off

Wyeth, John, and Brother Ltd., USA PA

U.S. Pat. Appl. Publ., 18 pp. so

CODEN: USXXCO

DTPatent

LΑ English

FAN.CNT 1				
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2004044024	A1	20040304	US 2003-629227	20030728
PRAI US 2002-399161P	P	20020729		

OS MARPAT 140:235704

GI

CN

Title compds. I [R1, R4 = H, (un) substituted alkyl, (un) substituted Ph, e.g., halo, OH, haloalkyl, etc.; R2 = H, (un)substituted alkyl, (un)substituted Ph, e.g., halo, NO2, CN, etc.; R3 = (un)substituted Ph, cycloheteroalkyl, heteroaryl, etc.], and their pharmaceutically acceptable salts were prepared For example, intramol. cyclization of compound II [R1 = H; R2 = 3-FC6H4; R3 = 5-bromopyrid-3-yl; R4 = CH3], e.g., prepared from Et 5-amino-1-methyl-4-pyrazolecarboxylate in 3-steps, afforded compound I [Rl = H; R2 = 3-FC6H4; R3 = 5-bromopyrid-3-yl; R4 = CH3] in 93% yield. In B7-1/CD28 binding inhibition assays, 75-examples of compds. I exhibited IC50 values ranging from 4-3000 nM, e.g., the IC50 value of compound I [R1 = H; R2 = 3-FC6H4; R3 = 5-bromopyrid-3-yl; R4 = CH3] was 20 nM. Of note, dihydrodipyrazolopyridinone I is useful for the immunotherapeutic treatment of transplant rejection and autoimmune diseases. 443146-92-7P 443146-93-8P 635324-71-9P 635324-72-0P 635324-73-1P 635324-75-3P 635324-76-4P 635324-79-7P 635324-82-2P 635324-84-4P 635324-85-5P 635324-87-7P 635324-90-2P 635324-92-4P 635324-93-5P 635324-94-6P 635324-95-7P 635324-96-8P 635324-97-9P 635324-98-0P 635324-99-1P 635325-03-0P 635325-05-2P 635325-06-3P 635325-07-4P 635325-09-6P 635325-11-0P 635325-19-8P 635325-20-1P 635325-21-2P 635325-23-4P 635325-25-6P 635325-27-8P 635325-28-9P 635325-29-0P 635325-30-3P 635325-31-4P 635325-32-5P 635325-34-7P 635325-35-8P 635325-36-9P 635325-37-0P 635325-38-1P 635325-77-8P 635325-95-0P 668481-76-3P 668481-77-4P 668481-78-5P 668481-79-6P 668481-80-9P 668481-81-0P 668481-82-1P 668481-83-2P 668481-84-3P 668481-85-4P 668481-86-5P 668481-87-6P 668481-88-7P 668481-89-8P 668481-90-1P 668481-91-2P 668481-92-3P 668481-93-4P 668481-94-5P 668481-96-7P 668481-97-8P 668481-98-9P 668481-99-0P 668482-00-6P 668482-01-7P 668482-02-8P 668482-03-9P 668482-04-0P 668482-06-2P 668482-07-3P

(Uses)
(preparation of dihydrodipyrazolopyridinones as B7-1/CD28 binding inhibitors for the immunotherapeutic treatment of organ transplant rejection)
443146-92-7 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

RN 443146-93-8 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME) CN

RN

635324-71-9 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-phenyl-CN4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

635324-72-0 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

RN 635324-73-1 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

RN 635324-75-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(2-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-76-4 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]-2-[4-(trifluoromethyl)-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$F_3$$
C N N Me

RN 635324-79-7 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(1,6-dihydro-6-oxo-3-pyridazinyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

$$rac{H}{N}$$
 $rac{H}{N}$ $rac{N}{N}$ $rac{M}{N}$ $rac{$

RN

635324-82-2 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-[4-(1,1-dimethylethyl)phenyl]-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

RN

635324-84-4 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-[4-(phenylmethoxy)phenyl]-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

635324-85-5 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-[1,1'-biphenyl]-4-yl-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN

635324-87-7 CAPLUS
Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN(CA INDEX NAME)

RN 635324-90-2 CAPLUS
CN Benzonitrile, 3-[2-(3-fluorophenyl)-1,2,3,6-tetrahydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-4-yl]- (9CI) (CA INDEX NAME)

RN 635324-92-4 CAPLUS
CN Benzoic acid, 3-[2-(3-fluorophenyl)-1,2,3,6-tetrahydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-4-yl]- (9CI) (CA INDEX NAME)

RN 635324-93-5 CAPLUS
CN Benzamide, 3-[2-(3-fluorophenyl)-1,2,3,6-tetrahydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-4-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & &$$

RN 635324-94-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(5-bromo-3-pyridinyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635324-95-7 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 635324-96-8 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-aminophenyl)-2-(4-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635324-97-9 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-1,6-dihydro-6-methyl-4-phenyl- (9CI) (CA INDEX NAME)

RN 635324-98-0 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-4-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

635324-99-1 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-pyridinyl)- (9CI) (CA INDEX NAME) CN

RN

635325-03-0 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3,5-dichlorophenyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN

635325-05-2 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-thienyl)- (9CI) (CA INDEX NAME) CN

RN

635325-06-3 CAPLUS Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-CN4-(3-methoxyphenyl)-6-methyl- (9CI) (CA INDEX NAME)

RN 635325-07-4 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(1,3-benzodioxol-5-yl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635325-09-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridine-3,4-dione, 2-(3-fluorophenyl)-1,2,5,6-tetrahydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635325-11-0 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(2,6-dimethyl-4-morpholinyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635325-19-8 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-phenyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-20-1 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-(phenylmethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-21-2 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,5-dihydro-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-23-4 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-2-(4-fluorophenyl)-1,6-dihydro-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-25-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-propyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-27-8 CAPLUS
CN Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

RN 635325-28-9 CAPLUS
CN Benzoic acid, 2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(lH)-yl]- (9CI)
(CA INDEX NAME)

RN 635325-29-0 CAPLUS
CN Benzoic acid, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-(9CI) (CA INDEX NAME)

RN 635325-30-3 CAPLUS
CN Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN 635325-31-4 CAPLUS
CN Benzoic acid, 2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN 635325-32-5 CAPLUS
CN Benzoic acid, 2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN 635325-34-7 CAPLUS
CN Benzoic acid, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-, methyl ester (9CI) (CA INDEX NAME)

RN 635325-35-8 CAPLUS
CN Benzoic acid, 2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

$$HO_2C$$
 H
 N
 N
 N
 N
 N
 Me

RN 635325-36-9 CAPLUS
CN Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-(9CI) (CA INDEX NAME)

$$HO_2C$$
 HO_2C
 HO_2

RN 635325-37-0 CAPLUS
CN Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-,
methyl ester (9CI) (CA INDEX NAME)

MeO-C
$$H$$
 N M

RN 635325-38-1 CAPLUS
CN Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-, methyl ester (9CI) (CA INDEX NAME)

RN 635325-77-8 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2(phenylmethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-95-0 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(2,4-difluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668481-76-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(5-bromo-3-pyridiny1)-2-(4-fluoropheny1)-1,6-dihydro-6-methy1- (9CI) (CA INDEX NAME)

RN 668481-77-4 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(5-bromo-3-pyridinyl)-1,6-dihydro-6-methyl-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 668481-78-5 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-(3-methylphenyl)-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 668481-79-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-(3-methylphenyl)-2-[3-methyl-5-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668481-80-9 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-bromophenyl)-1,6-dihydro-6-methyl-2-[3-methyl-5-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668481-81-0 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-bromophenyl)-1,6-dihydro-6-methyl-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 668481-82-1 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-(5-methyl-3-pyridinyl)-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 668481-83-2 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-(5-methyl-3-pyridinyl)-2-[3-methyl-5-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668481-84-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-2-(4-iodophenyl)-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668481-85-4 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-bromophenyl)-2-(3,5-dimethylphenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

668481-86-5 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-bromophenyl)-1,6-dihydro-6-methyl-2-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

668481-87-6 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3,5-dimethylphenyl)-1,6-dihydro-6-methyl-4-(3-methylphenyl)- (9CI) (CA INDEX NAME) CN

RN

668481-88-7 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3,5-dimethylphenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

RN

668481-89-8 CAPLUS Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(6-ethoxy-3-pyridazinyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

RN 668481-90-1 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3,5-dimethylphenyl)-1,6-dihydro-6-methyl-4-(4-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 668481-91-2 CAPLUS
CN Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 668481-92-3 CAPLUS
CN Benzoic acid, 4-[4-(3-bromophenyl)-3,6-dihydro-6-methyl-3oxodipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-chloro-, methyl ester
(9CI) (CA INDEX NAME)

RN 668481-93-4 CAPLUS
CN Benzoic acid, 4-[4-(3-bromophenyl)-3,6-dihydro-6-methyl-3oxodipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-chloro- (9CI) (CA INDEX

RN 668481-94-5 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-(4-nitrophenyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668481-96-7 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-aminophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668481-97-8 CAPLUS
CN 2-Thiophenecarboxylic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 668481-98-9 CAPLUS
CN 2-Thiophenecarboxylic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-4-

methyl- (9CI) (CA INDEX NAME)

RN 668481-99-0 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668482-00-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(methylsulfinyl)phenyl]- (9CI) (CA INDEX NAME)

RN

668482-01-7 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-[3-(phenylmethoxy)phenyl]-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX CN

$$\begin{array}{c|c} Ph-CH_2-O & H & N \\ \hline & N & N \\ \hline & N & N \\ \hline & N & Me \\ \hline & F_3C & N \\ \end{array}$$

RN

668482-02-8 CAPLUS
Benzoic acid, 4-[[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

MeO-C
$$CH_2$$
 N N N Me

668482-03-9 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-CN6-(2-hydroxyethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

F₃C
$$\stackrel{\text{H}}{\longrightarrow}$$
 $\stackrel{\text{N}}{\longrightarrow}$ $\stackrel{\text{N}}{\longrightarrow}$ $\stackrel{\text{CH}_2-\text{CH}_2-\text{OH}}{\longrightarrow}$

668482-04-0 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(2-fluoro[1,1'-biphenyl]-4-yl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN 668482-06-2 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,5-dihydro-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 668482-07-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(5-bromo-3-pyridinyl)-1,6-dihydro-6-methyl-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

OS GI

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ANSWER 2 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
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     2004:100816 CAPLUS
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DN
     140:163860
     Preparation of dihydrodipyrazolopyridinylbenzamide and -sulfonamide
ΤI
     inhibitors of B7-1
     Green, Neal Jeffrey; Xiang, Jason Shaoyun; Davies, Audrey Molina; Chen,
IN
     Lihren
     Wyeth, John, and Brother Ltd., USA
PΑ
     U.S. Pat. Appl. Publ., 19 pp.
SO
     CODEN: USXXCO
     Patent
DT
                                                                        16734190
LΑ
     English
FAN.CNT 1
                                           APPLICATION NO. DATE
     PATENT NO.
                      KIND DATE
                                                            20030728
                       Al
                            20040205
                                           US 2003-629276
    US 2004024008
ΡI
                            20020729
PRAI US 2002-399146P
                       P
     MARPAT 140:163860
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$$R^3$$
 $-X-NR^4R^5$
 N
 N
 N
 R^6

The title compds. [I; X = CO, SO2; R1, R2 = H, alkyl, haloalkyl, cycloalkyl, etc.; R3 = H, F, Cl, Br, I; R4, R5 = H, NH2, (CH2)2O(CH2)2NH2, etc.; or NR4R5 = (un)substituted 5-7 membered ring optionally containing one double bond, benzofused ring or an addnl. heteroatom selected from O, (un)substituted NH, S; R6 = (un)substituted Ph, cycloheteroalkyl, heteroaryl], useful for the immunotherapeutic treatment of transplant rejection or autoimmune disease, were prepared E.g., a multi-step synthesis of II which showed IC50 of 54 nM in test for B7-1/CD28 binding inhibition, was given. The pharmaceutical composition comprising the compound I is claimed.

T

II

RN 635324-83-3 CAPLUS
CN Benzenesulfonamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

$$\begin{array}{c|c} \circ & & & \\ H_2N-S & & & \\ \bullet & & \\ \bullet$$

RN 635325-27-8 CAPLUS
CN Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

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635325-39-2P 635325-40-5P 635325-41-6P
           635325-42-7P 635325-43-8P 635325-44-9P
           635325-45-0P 635325-46-1P 635325-47-2P
           635325-48-3P 635325-49-4P 635325-50-7P
           635325-51-8P 635325-52-9P 635325-53-0P
           635325-54-1P 635325-55-2P 635325-57-4P
           635325-58-5P 635325-59-6P 635325-60-9P
           635325-61-0P 635325-62-1P 635325-63-2P
           635325-64-3P 635325-65-4P 635325-66-5P
           635325-67-6P 635325-68-7P 635325-69-8P
            654679-05-7P 654679-15-9P 654679-21-7P
           654679-27-3P 654679-32-0P 654679-41-1P
            654679-48-8P 654679-54-6P 654679-59-1P
            654679-71-7P 654679-76-2P 654679-91-1P
           654679-98-8P 654680-10-1P 654680-61-2P
            654680-66-7P 654680-75-8P 654680-80-5P
            654680-93-0P 654680-98-5P 654681-03-5P
            654681-08-0P 654681-13-7P 654681-17-1P
            654681-25-1P 654681-35-3P 654681-38-6P
            654681-43-3P 654681-45-5P 654681-46-6P
            654681-49-9P 654681-52-4P 654681-55-7P
            654681-60-4P 654681-63-7P 654681-68-2P
            654681-70-6P 654681-75-1P 654681-78-4P
            654681-81-9P 654681-84-2P 654681-86-4P
            654681-88-6P 654681-90-0P 654681-92-2P
            654681-94-4P 654681-96-6P 654681-98-8P
            654682-02-7P 654682-04-9P 654682-06-1P
            654682-08-3P 654682-10-7P 654682-12-9P
            654682-14-1P 654682-17-4P 654682-20-9P
            654682-22-1P 654682-24-3P 654682-27-6P
            654682-28-7P 654682-30-1P 654682-32-3P
            654682-34-5P 654682-37-8P 654682-40-3P
            654682-42-5P 654682-44-7P 654682-46-9P
            654682-48-1P
            RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
            (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
             (Uses)
                    (preparation of dihydrodipyrazolopyridinylbenzamide and -sulfonamide
                    inhibitors of B7-1/CD28 binding)
            635325-39-2 CAPLUS
RN
            Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-
CN
            \label{lem:condition} (\texttt{trifluoromethyl}) \, \texttt{phenyl}] \, \texttt{dipyrazolo[3,4-b:3',4'-d]} \, \texttt{pyridin-2(1H)-yl]-N-(3-b)} \, \text{where} \, \text{trifluoromethyl} \, \text{
            hydroxypropyl) - (9CI) (CA INDEX NAME)
```

HO-
$$(CH_2)_3$$
-NH-C H N N Me

(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3-methoxypropyl)- (9CI) (CA INDEX NAME)

MeO - (CH₂)₃ - NH - C
$$\stackrel{\text{H}}{\underset{\text{N}}{\parallel}}$$
 $\stackrel{\text{N}}{\underset{\text{N}}{\parallel}}$ $\stackrel{\text{N}}{\underset{\text{N}}{\parallel}}$ $\stackrel{\text{Me}}{\underset{\text{N}}{\parallel}}$

RN 635325-41-6 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3-methoxypropyl)- (9CI) (CA INDEX NAME)

MeO- (CH₂)₃-NH-C
$$\stackrel{\text{H}}{\underset{\text{N}}{\bigvee}}$$
 $\stackrel{\text{N}}{\underset{\text{N}}{\bigvee}}$ $\stackrel{\text{N}}{\underset{\text{N}}{\bigvee}}$ $\stackrel{\text{N}}{\underset{\text{N}}{\bigvee}}$

RN 635325-42-7 CAPLUS
CN Piperazine, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-4-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ N & & & \\ N & & \\ N & & \\ \end{array}$$

RN 635325-43-8 CAPLUS
CN Morpholine, 4-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

RN 635325-44-9 CAPLUS
CN Morpholine, 4-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluorobenzoyl]- (9CI) (CA INDEX NAME)

RN 635325-45-0 CAPLUS
CN Morpholine, 4-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

RN 635325-46-1 CAPLUS
CN Pyrrolidine, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

RN 635325-47-2 CAPLUS
CN Pyrrolidine, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

RN 635325-48-3 CAPLUS
CN D-Proline, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl], methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-49-4 CAPLUS
CN D-Proline, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-50-7 CAPLUS
CN D-Proline, 1-[2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-51-8 CAPLUS CN L-Proline, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-52-9 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 635325-53-0 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 635325-54-1 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 635325-55-2 CAPLUS
CN Isoquinoline, 2-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

$$\bigcap_{N-C}\bigcap_{N-M}$$

RN 635325-57-4 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(3,4-dihydroxyphenyl)methyl]- (9CI) (CA INDEX NAME)

RN 635325-58-5 CAPLUS
CN Benzamide, 2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(3,4-dihydroxyphenyl)methyl]- (9CI) (CA INDEX NAME)

RN 635325-59-6 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(4-hydroxy-3-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

RN 635325-60-9 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(lH)-yl]-N-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

HO-
$$CH_2$$
- CH_2

NH- C

N

N

Me

RN 635325-61-0 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-62-1 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HO-CH}_2 & \text{NH-C} & \text{N} & \text{N} \\ \hline \\ \text{N} & \text{N} & \text{N} \\ \hline \end{array}$$

RN 635325-63-2 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-64-3 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(methoxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN

635325-65-4 CAPLUS Benzoic acid, 3-[[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

MeO-C
$$NH-C$$
 $NH-C$ N

635325-66-5 CAPLUS RN

Benzamide, N-(3-acetylphenyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN(CA INDEX NAME)

635325-67-6 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME) CN

635325-68-7 CAPLUS RN

Benzamide, 2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-69-8 CAPLUS
CN Morpholine, 4-[5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluorobenzoyl]- (9CI) (CA INDEX NAME)

RN 654679-05-7 CAPLUS
CN Benzoic acid, 4-chloro-3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

RN 654679-15-9 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

RN

654679-21-7 CAPLUS

Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2,2-dimethoxyethyl)-N-methyl- (9CI) (CA INDEX NAME) CN

RN

654679-27-3 CAPLUS Thiazolidine, 3-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

654679-32-0 CAPLUS RN

Thiomorpholine, 4-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

RN

654679-41-1 CAPLUS
Benzamide, N-(cyclopropylmethyl)-3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN (CA INDEX NAME)

RN 654679-48-8 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2-hydroxyethyl)-N-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} & \text{N} \\ & \text{HO-CH}_2\text{-CH}_2\text{-N-C} & \text{N} \\ & \text{N} & \text{N} \\ & \text{N} & \text{N} \end{array}$$

RN 654679-54-6 CAPLUS
CN 1H-Indole-3-carboxylic acid, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 654679-59-1 CAPLUS
CN Benzamide, N-[(4-aminophenyl)methyl]-3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

RN 654679-71-7 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2-hydroxypropyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \text{O} & \text{H} & \text{N} \\ \text{Me-CH-CH}_2\text{-NH-C} & \text{N} & \text{N} & \text{N} \\ \end{array}$$

RN 654679-76-2 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & H & N \\ H & N & N \\ \hline \\ O & N & Me \\ \end{array}$$

RN 654679-91-1 CAPLUS
CN 2-Pyrrolidinemethanol, 1-[2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl], (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

654679-98-8 CAPLUS Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

654680-10-1 CAPLUS RN

4-Piperidinecarboxylic acid, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-, methyl ester (9CI) (CA INDEX NAME) CN

$$\begin{array}{c|c} & & & \\ & & & \\ N & - C & \\ \hline & & \\ N & \\ \end{array}$$

654680-61-2 CAPLUS RN

3-Piperidinemethanol, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

654680-66-7 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(4-hydroxybutyl)- (9CI) (CA INDEX NAME) CN

RN 654680-75-8 CAPLUS
CN Benzamide, N-(5-aminopentyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

RN 654680-80-5 CAPLUS
CN Morpholine, 4-[2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

RN 654680-93-0 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(lH)-yl]-N-(5,6,7,8-tetrahydro-5-hydroxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 654680-98-5 CAPLUS
CN Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, hydrazide (9CI) (CA INDEX NAME)

RN 654681-03-5 CAPLUS
CN Glycine, N-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl], methyl ester (9CI) (CA INDEX NAME)

RN 654681-08-0 CAPLUS
CN Benzamide, N-[2-[2-(2-aminoethoxy)ethoxy]ethy1]-3-[3,6-dihydro-6-methy1-3-oxo-4-[3-(trifluoromethy1)pheny1]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-y1]- (9CI) (CA INDEX NAME)

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PAGE 1-B

RN 654681-13-7 CAPLUS
CN Benzamide, N-(3,4-difluorophenyl)-3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

RN 654681-17-1 CAPLUS
CN Benzoic acid, 3-[[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 654681-25-1 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

654681-35-3 CAPLUS RN4-Piperidinecarboxylic acid, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

654681-38-6 CAPLUS RN

Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME) CN

HO-
$$CH_2$$
- CH_2

NH- C

NH- C

NH- C

NH- C

RN

654681-43-3 CAPLUS
Piperidine, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-3-methyl- (9CI) (CA INDEX NAME) CN

654681-45-5 CAPLUS

3-Piperidinecarboxamide, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-N,N-diethyl- (9CI) (CA INDEX NAME) CN

$$\begin{array}{c|c} O & O & H & N \\ \hline Et_2N-C & N & N & N \\ \hline N & N & N \\ \hline N & N & N & N \\ N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N & N \\ \hline N & N & N \\ N & N & N \\ \hline N & N & N \\ N & N & N \\ \hline N & N & N$$

RN654681-46-6 CAPLUS

4-Piperidinol, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-CN (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

654681-49-9 CAPLUS RN

Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(4methoxyphenyl) methyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{O} & \text{H} & \text{N} \\ \text{CH}_2-\text{NH}-\text{C} & \text{N} & \text{N} \\ \text{O} & \text{N} & \text{N} \end{array}$$

654681-52-4 CAPLUS RN

Benzamide, N-(2-cyanoethyl)-3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl) phenyl] dipyrazolo[3,4-b:3',4'-d] pyridin-2(1H)-yl]-Nmethyl- (9CI) (CA INDEX NAME)

RN 654681-55-7 CAPLUS
CN Benzamide, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

HO-
$$CH_2$$
- CH_2

NH- C

N

N

N

N

N

N

CF3

RN 654681-60-4 CAPLUS CN D-Proline, 1-[2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 654681-63-7 CAPLUS
CN Benzamide, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 654681-68-2 CAPLUS

Benzamide, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

654681-70-6 CAPLUS RN

Benzamide, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-[4-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME) CN

654681-75-1 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN(CA INDEX NAME)

$$H_2N-C$$
 H_2N-C
 H

RN

654681-78-4 CAPLUS
Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3-CNhydroxyphenyl) - (9CI) (CA INDEX NAME)

RN 654681-81-9 CAPLUS
CN Benzamide, N-(2-cyanoethyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ & \text{NC-CH}_2\text{-CH}_2\text{-N-C} \\ & \text{N} \\ & \text$$

RN 654681-84-2 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

RN 654681-86-4 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)

RN

654681-88-6 CAPLUS
Benzamide, N-(cyclopropylmethyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN(CA INDEX NAME)

RN

654681-90-0 CAPLUS Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2hydroxypropyl) - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \text{O} \\ \text{Me-CH-CH}_2 - \text{NH-C} & \text{H} & \text{N} \\ \\ \text{N} & \text{N} & \text{Me} \end{array}$$

654681-92-2 CAPLUS RN

Thiomorpholine, 4-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

654681-94-4 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 654681-96-6 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-3-pyridinyl- (9CI) (CA INDEX NAME)

RN 654681-98-8 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2,2-dimethoxyethyl)-N-methyl- (9CI) (CA INDEX NAME)

RN 654682-02-7 CAPLUS
CN Benzamide, N-(3,4-difluorophenyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

RN 654682-04-9 CAPLUS
CN Thiazolidine, 3-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(lH)-yl]benzoyl](9CI) (CA INDEX NAME)

RN 654682-06-1 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(hydroxymethyl)-2-methylphenyl]- (9CI) (CA INDEX NAME)

RN 654682-08-3 CAPLUS
CN Benzamide, N-(3-amino-3-oxopropyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-methyl- (9CI) (CA INDEX NAME)

RN

654682-10-7 CAPLUS
Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[2-CN(hydroxymethyl)phenyl] - (9CI) (CA INDEX NAME)

$$CH_2-OH$$
 O
 $NH-C$
 $NH-C$

654682-12-9 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[4-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

654682-14-1 CAPLUS RN

3-Piperidinecarboxamide, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-N,N-diethyl- (9CI) (CA INDEX NAME) CN

RN654682-17-4 CAPLUS

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(dimethylamino)propyl]- (9CI) (CA INDEX NAME)

654682-20-9 CAPLUS

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(4fluorophenyl) methyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

RN

654682-22-1 CAPLUS

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2-CN hydroxyethyl) - N-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ & \text{II} \\ \text{HO-CH}_2\text{-CH}_2\text{-N-C} \\ & \text{N} \\ & \text{N} \\ & \text{Me} \\ & \text{N} \\ & \text{Me} \\ & \text{N} \\ & \text{N} \\ & \text{Me} \\ & \text{N} \\ &$$

654682-24-3 CAPLUS RN

4-Piperidinol, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

RN 654682-27-6 CAPLUS
CN 3-Piperidinol, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

HO N C
$$\mathbb{N}$$
 \mathbb{N} \mathbb{N} \mathbb{N} \mathbb{N} \mathbb{N} \mathbb{N} \mathbb{N} \mathbb{N}

RN 654682-28-7 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(5-hydroxypentyl)- (9CI) (CA INDEX NAME)

HO-
$$(CH_2)_5$$
-NH-C

N
N
N
Me

RN 654682-30-1 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3,4-dihydroxyphenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \text{O} & \text{H} & \text{N} \\ \hline & \text{N} & \text{N} & \text{Me} \\ \hline & \text{O} & \text{N} & \text{Me} \\ \hline & \text{O} & \text{N} & \text{N} & \text{Me} \\ \hline & \text{O} & \text{N} & \text{N} & \text{N} \\ \hline & \text{O} & \text{N} \\ \hline & \text{O} & \text{N} \\ \hline & \text{O} & \text{N} & \text{N} \\ \hline & \text{O} & \text{N} & \text{N} \\ \hline & \text{O} & \text{$$

RN 654682-32-3 CAPLUS

CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

RN 654682-34-5 CAPLUS

CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(1-hydroxypropyl)phenyl]- (9CI) (CA INDEX NAME)

RN 654682-37-8 CAPLUS

CN Benzenesulfonamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(5-hydroxypentyl)- (9CI) (CA INDEX NAME)

HO-
$$(CH_2)_5$$
-NH-S N Me

RN 654682-40-3 CAPLUS

CN Benzenesulfonamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 654682-42-5 CAPLUS
CN Benzenesulfonamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} \\$$

RN 654682-44-7 CAPLUS
CN Glycine, N-[[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]phenyl]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 654682-46-9 CAPLUS
CN Benzenesulfonamide, N-(cyclopropylmethyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl](9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-NH^{-1}S & H & N \\ \hline \\ O & N & N \\ \hline \\ O & F_3C \\ \end{array}$$

RN 654682-48-1 CAPLUS

CN Glycine, N-[[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)yl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

IT 654682-52-7P 654682-55-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of dihydrodipyrazolopyridinylbenzamide and -sulfonamide inhibitors of B7-1/CD28 binding)

RN 654682-52-7 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridine-1(2H)-carboxylic acid,
2-[4-[[[(1,1-dimethylethoxy)carbonyl]amino]sulfonyl]phenyl]-3,6-dihydro-6methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI)
(CA INDEX NAME)

RN 654682-55-0 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridine-1(2H)-carboxylic acid,
3,6-dihydro-2-[4-[[(5-hydroxypentyl)amino]sulfonyl]phenyl]-6-methyl-3-oxo4-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

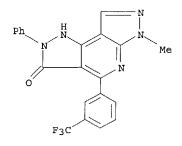
ΑN 2003:427773 CAPLUS DN 140:42073 TI Structure-activity studies of a series of dipyrazolo[3,4-b:3',4'-d]pyridin-3-ones binding to the immune regulatory protein B7.1 AU Green, Neal J.; Xiang, Jason; Chen, Jing; Chen, Lihren; Davies, Audrey M.; Erbe, Dave; Tam, Steve; Tobin, James F. CS Department of Chemical Sciences, Wyeth Research, Cambridge, MA, 02140, USA so Bioorganic & Medicinal Chemistry (2003), 11(13), 2991-3013 CODEN: BMECEP; ISSN: 0968-0896 PΒ Elsevier Science Ltd. \mathtt{DT} Journal LΑ English GI

I

AB The interaction of co-stimulatory mols. on T cells with B7 mols. on antigen presenting cells plays an important role in the activation of naive T cells. Consequently, agents that disrupt these interactions should have applications in treatment of transplant rejection as well as autoimmune diseases. To this end, specific small mol. inhibitors of human B7.1 were identified and characterized. Herein, we report the identification of potent small mol. inhibitors of the $\overline{{\tt B7.1-CD28}}$ interaction. In a high-throughput screen we identified several leads that prevented the interaction of B7.1 with CD28 with activities in the nanomolar to low micromolar range. One of these, the dihydrodipyrazolopyridinone I, was subsequently shown to bind the V-like domain of human B7.1 at equimolar stoichiometry. With this as a starting point, we report here the synthesis and initial in vitro structure-activity relationships of a series of these compds. 635324-71-9 635325-69-8 635325-95-0 RL: PAC (Pharmacological activity); BIOL (Biological study) (preparation and structure-activity relationship of a series of dipyrazolo[3,4-b:3',4'-d]pyridin-3-ones as inhibitors of the B7.1-CD28 interaction in T cells) RN 635324-71-9 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-phenyl-

4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



CN

RN 635325-69-8 CAPLUS
CN Morpholine, 4-[5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluorobenzoyl]- (9CI) (CA INDEX NAME)

RN 635325-95-0 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(2,4-difluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

IT 443146-92-7P 635324-87-7P 635324-90-2P

635324-95-7P 635325-20-1P 635325-21-2P

635325-27-8P 635325-28-9P 635325-29-0P

635325-32-5P 635325-35-8P 635325-36-9P

635325-38-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation and structure-activity relationship of a series of dipyrazolo[3,4-b:3',4'-d]pyridin-3-ones as inhibitors of the B7.1-CD28 interaction in T cells)

RN 443146-92-7 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Cl} & \text{N} & \text{N} \\ \hline & \text{N} & \text{N} \\ \hline & \text{N} & \text{N} \\ \hline & \text{F}_3\text{C} & \\ \end{array}$$

635324-87-7 CAPLUS

RN

CN Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

635324-90-2 CAPLUS RN

Benzonitrile, 3-[2-(3-fluorophenyl)-1,2,3,6-tetrahydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-4-yl]- (9CI) (CA INDEX NAME) CN

RN

635324-95-7 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-CN 6-methyl-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

635325-20-1 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-(phenylmethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

RN

635325-21-2 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,5-dihydro-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

RN

635325-27-8 CAPLUS
Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN(CA INDEX NAME)

RN

635325-28-9 CAPLUS Benzoic acid, 2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

635325-29-0 CAPLUS
Benzoic acid, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl) phenyl] dipyrazolo[3,4-b:3',4'-d] pyridin-2(1H)-yl]-2fluoro- (9CI) (CA INDEX NAME)

635325-32-5 CAPLUS
Benzoic acid, 2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN

635325-35-8 CAPLUS Benzoic acid, 2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

$$HO_2C$$
 HO_2C
 HO_2

RN 635325-36-9 CAPLUS

CNBenzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro- (9CI) (CA INDEX NAME)

$$HO_2C$$
 N
 N
 N
 N
 N
 N
 N
 N
 N

635325-38-1 CAPLUS Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2fluoro-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & F & N & N \\ \hline & N & N & Me \\ \hline & N & N & Me \\ \hline & CF_3 & Me \\ \end{array}$$

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443146-93-8P 635324-72-0P 635324-73-1P
     635324-74-2P 635324-75-3P 635324-76-4P
     635324-77-5P 635324-79-7P 635324-82-2P
     635324-83-3P 635324-84-4P 635324-85-5P
     635324-86-6P 635324-88-8P 635324-91-3P
     635324-92-4P 635324-93-5P 635324-94-6P
     635324-96-8P 635324-97-9P 635324-98-0P
     635324-99-1P 635325-03-0P 635325-05-2P
     635325-06-3P 635325-07-4P 635325-11-0P
     635325-13-2P 635325-19-8P 635325-23-4P
     635325-25-6P 635325-30-3P 635325-31-4P
     635325-34-7P 635325-37-0P 635325-39-2P
     635325-40-5P 635325-41-6P 635325-42-7P
     635325-43-8P 635325-44-9P 635325-45-0P
     635325-46-1P 635325-47-2P 635325-48-3P
     635325-49-4P 635325-50-7P 635325-51-8P
     635325-52-9P 635325-53-0P 635325-54-1P
     635325-55-2P 635325-56-3P 635325-57-4P
     635325-58-5P 635325-59-6P 635325-60-9P
     635325-61-0P 635325-62-1P 635325-63-2P
     635325-64-3P 635325-65-4P 635325-66-5P
     635325-67-6P 635325-68-7P 635325-77-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation)
        (preparation and structure-activity relationship of a series of
        dipyrazolo[3,4-b:3',4'-d]pyridin-3-ones as inhibitors of the B7.1-CD28
        interaction in T cells)
RN
     443146-93-8 CAPLUS
CN
    Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-
     6-methyl-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME)
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RN 635324-72-0 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)
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RN 635324-73-1 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-74-2 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-chloro-4-fluorophenyl)1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-75-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(2-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-76-4 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-[3(trifluoromethyl)phenyl]-2-[4-(trifluoromethyl)-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 635324-77-5 CAPLUS
CN 2-Thiophenecarboxylic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-5-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CO}_2\text{H} & \text{H} & \text{N} \\ \text{N} & \text{N} & \text{N} \\ \text{Me} & \text{O} & \text{N} & \text{N} \end{array}$$

RN 635324-79-7 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(1,6-dihydro-6-oxo-3-pyridazinyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-82-2 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-[4-(1,1-dimethylethyl)phenyl]-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl](9CI) (CA INDEX NAME)

RN 635324-83-3 CAPLUS
CN Benzenesulfonamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

RN 635324-84-4 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-[4-(phenylmethoxy)phenyl]-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \operatorname{Ph-CH_2-O} & & & \\$$

RN 635324-85-5 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-[1,1'-biphenyl]-4-yl-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-86-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-2-[4-(hydroxymethy1)pheny1]-6-methy1-4-[3-(trifluoromethy1)pheny1]- (9CI) (CA INDEX NAME)

RN 635324-88-8 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-91-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-bromophenyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635324-92-4 CAPLUS CN Benzoic acid, 3-[2-(3-fluorophenyl)-1,2,3,6-tetrahydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-4-yl]- (9CI) (CA INDEX NAME)

635324-93-5 CAPLUS

Benzamide, 3-[2-(3-fluorophenyl)-1,2,3,6-tetrahydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-4-yl]- (9CI) (CA INDEX NAME) CN

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN

635324-94-6 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(5-bromo-3-pyridinyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME) CN

RN

635324-96-8 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-aminophenyl)-2-(4-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME) CN

635324-97-9 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-1,6-dihydro-6-methyl-4-phenyl- (9CI) (CA INDEX NAME) CN

RN 635324-98-0 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-4-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME) CN

RN

635324-99-1 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-pyridinyl)- (9CI) (CA INDEX NAME) CN

RN 635325-03-0 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3,5-dichlorophenyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN

635325-05-2 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-thienyl)- (9CI) (CA INDEX NAME) CN

RN 635325-06-3 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-4-(3-methoxyphenyl)-6-methyl- (9CI) (CA INDEX NAME)

RN 635325-07-4 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(1,3-benzodioxol-5-yl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 635325-11-0 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(2,6-dimethyl-4-morpholinyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635325-13-2 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-1,6-dihydro-1,6-dimethyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-phenyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-23-4 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-2-(4-fluorophenyl)-1,6-dihydro-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-25-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-propyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-30-3 CAPLUS
CN Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, methyl ester (9CI) (CA INDEX NAME)

MeO-C
$$H$$
 N M

RN 635325-31-4 CAPLUS

CNBenzoic acid, 2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN

635325-34-7 CAPLUS Benzoic acid, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2fluoro-, methyl ester (9CI) (CA INDEX NAME)

635325-37-0 CAPLUS Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl) phenyl] dipyrazolo[3,4-b:3',4'-d] pyridin-2(1H)-yl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & & \\ MeO-C & & & & \\ \hline & N & & \\ \hline & N & & \\ \hline & N & &$$

635325-39-2 CAPLUS RN

CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl) phenyl] dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3-hydroxypropyl)- (9CI) (CA INDEX NAME)

HO-
$$(CH_2)_3$$
-NH-C

RN 635325-40-5 CAPLUS

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3-methoxypropyl)- (9CI) (CA INDEX NAME) CN

MeO- (CH₂)₃-NH-C
$$\stackrel{\text{H}}{\underset{\text{N}}{\text{H}}}$$
 $\stackrel{\text{N}}{\underset{\text{N}}{\text{N}}}$ $\stackrel{\text{N}}{\underset{\text{N}}{\text{Me}}}$

RN635325-41-6 CAPLUS

Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3-CNmethoxypropyl) - (9CI) (CA INDEX NAME)

MeO- (CH₂)₃-NH-C
$$\stackrel{\text{H}}{\underset{\text{N}}{|}}$$
 $\stackrel{\text{H}}{\underset{\text{N}}{|}}$ $\stackrel{\text{N}}{\underset{\text{N}}{|}}$ $\stackrel{\text{Me}}{\underset{\text{N}}{|}}$

RN

635325-42-7 CAPLUS
Piperazine, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-4-methyl- (9CI) (CA INDEX NAME)

635325-43-8 CAPLUS Morpholine, 4-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

$$\bigcap_{N} \bigcap_{C} \bigcap_{N} \bigcap_{N$$

635325-44-9 CAPLUS
Morpholine, 4-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluorobenzoyl]- (9CI) (CA INDEX NAME)

RN

635325-45-0 CAPLUS Morpholine, 4-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

RN

635325-46-1 CAPLUS
Pyrrolidine, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

RN 635325-47-2 CAPLUS
CN Pyrrolidine, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

RN 635325-48-3 CAPLUS
CN D-Proline, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl], methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-49-4 CAPLUS CN D-Proline, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-50-7 CAPLUS
CN D-Proline, 1-[2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-51-8 CAPLUS
CN L-Proline, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-52-9 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 635325-53-0 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(lH)-yl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Ph} & \text{CH}_2 - \text{NH} - \text{C} \\ \hline \\ \text{O} \\ \hline \\ \text{F}_3 \text{C} \\ \end{array}$$

RN 635325-54-1 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ & & \text{II} \\ \text{Ph-CH}_2 - \text{N-C} \\ & & \text{N} \\ \end{array}$$

RN 635325-55-2 CAPLUS
CN Isoquinoline, 2-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ N & & \\ \hline \end{array}$$

RN 635325-56-3 CAPLUS

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(3,4-dihydroxyphenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \\ \text{O} & \\ \text{CH}_2 - \text{NH} - \text{C} \\ \end{array}$$

RN 635325-57-4 CAPLUS

CN

Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3- $(trifluoromethyl)\,phenyl]\,dipyrazolo\,[3,4-b:3',4'-d]\,pyridin-2\,(1H)\,-yl]\,-N-\,[\,(3,4-b:3',4'-d]\,pyridin-2\,(2H)\,-yl]\,-N-\,[\,(3,4-b:3',4'-d]\,-yl]\,-N-\,[\,(3,4-b:3',4'-d]\,-yl]\,-N-\,[\,(3,4-b:3',4'-d]\,-yl]\,-N-\,[\,(3,4-b:3',4'-d]\,-yl]\,-N-\,[\,(3,4-b:3',4'-d]\,-yl]\,-N-\,[\,(3,4-b:3',4'-d]\,-yl]\,-N-\,[\,(3,4-b:3',4'-d]\,-yl]\,-N-\,[\,(3,4-b:3',4'$ dihydroxyphenyl)methyl] - (9CI) (CA INDEX NAME)

HO CH₂-NH-C
$$\stackrel{\text{H}}{\longrightarrow}$$
 $\stackrel{\text{N}}{\longrightarrow}$ $\stackrel{$

RN 635325-58-5 CAPLUS

Benzamide, 2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(3,4dihydroxyphenyl) methyl] - (9CI) (CA INDEX NAME)

RN

635325-59-6 CAPLUS Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(4hydroxy-3-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{OMe} \\ \mathsf{HO} \\ & \mathsf{CH}_2 - \mathsf{NH} - \mathsf{C} \\ & \mathsf{N} \\ & \mathsf{$$

RN

635325-60-9 CAPLUS
Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME) CN

$$\begin{array}{c|c} \text{HO-CH}_2\text{-CH}_2 \\ \hline \\ \text{NH-C} \\ \hline \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{Me} \\ \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \\ \text{N} \\ \\ \text{$$

RN

635325-61-0 CAPLUS
Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME) CN

$$\begin{array}{c|c} \text{HO-CH}_2\text{-CH}_2 \\ \hline \\ \text{NH-C} \\ \hline \\ \text{N} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{Me} \\ \\ \text{CF}_3 \\ \end{array}$$

635325-62-1 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN635325-63-2 CAPLUS

Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-64-3 CAPLUS

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN $(\texttt{trifluoromethyl}) \, \texttt{phenyl}] \, \texttt{dipyrazolo} \, [\texttt{3,4-b:3',4'-d}] \, \texttt{pyridin-2(1H)-yl}] \, - \texttt{N-[3-hearthyl]} \, + \texttt{N-[3-hea$ (methoxymethyl)phenyl] - (9CI) (CA INDEX NAME)

RN

635325-65-4 CAPLUS Benzoic acid, 3-[[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

635325-66-5 CAPLUS
Benzamide, N-(3-acetylphenyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN (CA INDEX NAME)

RN 635325-67-6 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-68-7 CAPLUS
CN Benzamide, 2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-77-8 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-(phenylmethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-09-6 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridine-3,4-dione, 2-(3-fluorophenyl)-1,2,5,6-tetrahydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635325-22-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,5-dihydro1-(phenylmethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-24-5 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-2-(4-fluorophenyl)-1,6-dihydro-1-(phenylmethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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DN 137:103581

Small molecule ligands define a binding site on the immune regulatory TΙ protein B7.1

ΑU Erbe, David V.; Wang, Suyue; King, Yuzhe; Tobin, James F. CS

Wyeth Research, Cambridge, MA, 02140, USA

Journal of Biological Chemistry (2002), 277(9), 7363-7368 SO CODEN: JBCHA3; ISSN: 0021-9258

PB American Society for Biochemistry and Molecular Biology

DTJournal

LΑ English

AΒ The interaction of co-stimulatory mols. on T cells with B7 mols. on antigen presenting cells plays an important role in the activation of naive T cells. Consequently, agents that disrupt these interactions should have applications in treatment of transplant rejection as well as autoimmune diseases. To this end, specific small mol. inhibitors of human B7.1 were identified and characterized. These compds. inhibit the binding of B7.1 to both CD28 and CTLA4. Both classes of compds. appear to bind the same site, a relatively small portion of the GFCC'C'' face of the N-terminal V-set domain of human B7.1, not present in the homologous B7.2 or even mouse B7.1. This site may represent a rare hot spot for small mol. antagonist design of inhibitors of cell-cell interactions, whose ligands may yield leads for the development of novel immunomodulatory medicines.

ΙT 443146-92-7 443146-93-8

RL: PAC (Pharmacological activity); BIOL (Biological study) (small mol. ligands define a binding site on the immune regulatory protein B7.1)

RN 443146-92-7 CAPLUS

CNDipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 443146-93-8 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-CN 6-methyl-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

T.4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1998:131636 CAPLUS

DN 128:192869

Synthesis of β -D-ribonucleosides derived from dipyrazolo[3,4-b:3'4'-ΤI d]pyridin-3-one system

Bernardino, Alice M. R.; Nogueira, Christiane M.; de O. Lepesch, Carla M.; AII Gomes, Claudia R. B.; Schmitz, Francis J.; Romeiro, Gilberto A.; de S. Pereira, Helena; de P. P. Frughlhetti, Isabel C.; de Oliveira, Mara R. P.; de Souza, maria C. B. V.; Lee, Marietta Y. W. T.; Chaves, Salma A.; Ferreira, Vitor F.

Departamento de Quimica Organica, Instituto de Quimica, Universidade CS

Federal Fluminense, Niteroi, 24020-150, Brazil Heterocyclic Communications (1997), 3(6), 527-534 SO CODEN: HCOMEX; ISSN: 0793-0283

PΒ Freund Publishing House Ltd.

DTJournal

LА English

The new ribonucleosides 8-methyl-2,6-diphenyl-5-(2,3,5-tri-0-benzoyl-AB β -D-ribofuranosyl)-2H,6H-dipyrazolo[3,4-b:3'4'-d]pyridin-3(5H)-one and 8-methyl-2-(p-nitrophenyl)-6-phenyl-5-(2,3,5-tri-O-benzoyl- β -Dribofuranosyl) -2H, 6H-dipyrazolo[3,4-b:3'4'-d]pyridin-3(5H)-one were prepared from stannic chloride-catalyzed ribosylations of the corresponding heterocycles. Attempts of de-O-benzoylation failed to give the free ribosides. The effect of these compds. on the catalytic activities of reverse transcriptase from recombinant immunodeficiency virus type 1 was evaluated. Some compds. inhibited the RNA dependent DNA polymerase activity of the enzyme by more than 50% at a concentration of 70 $\mu M. \label{eq:model}$ contrast, human placental DNA polymerase activities α and ϵ were unaffected by this concentration The structures of the nucleosides are supported by 1D and 2D-NMR techniques (nOdes, HMBC and HMQC expts.). 81153-40-4P 203719-80-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (preparation of ribonucleosides derived from a dipyrazolopyridinone system)

81153-40-4 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-8-methyl-2,6diphenyl- (9CI) (CA INDEX NAME)

RN 203719-80-6 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-8-methyl-2-(4nitrophenyl)-6-phenyl- (9CI) (CA INDEX NAME)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 6 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN AN 1982:142751 CAPLUS 96:142751 Tricyclic heteroatomic ring systems. III. Synthesis of 1H,6H-dipyrazolo[3,4-b:3',4'-d]pyridin-3-ones TI Khan, Misbahul A.; Pedrotti, Francisco Secao Quim., Inst. Mil. Eng., Rio de Janeiro, 22290, Brazil Monatshefte fuer Chemie (1982), 113(1), 123-7 ΑU CS SO CODEN: MOCMB7; ISSN: 0026-9247 DT Journal LΑ English OS CASREACT 96:142751 GT

IT 81153-31-3P 81153-32-4P 81153-33-5P 81153-34-6P 81153-35-7P 81153-36-8P 81153-37-9P 81153-38-0P 81153-39-1P 81153-41-5P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
RN 81153-31-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6,8-dimethyl-(9CI) (CA INDEX NAME)

RN 81153-32-4 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-8-phenyl-(9CI) (CA INDEX NAME)

RN 81153-33-5 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6,8-diphenyl-(9CI) (CA INDEX NAME)

RN 81153-34-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-8-methyl-6-phenyl(9CI) (CA INDEX NAME)

RN 81153-35-7 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1,6,8-trimethyl-(9CI) (CA INDEX NAME)

RN 81153-36-8 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1,6-dimethyl-8-phenyl- (9CI) (CA INDEX NAME)

RN 81153-37-9 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1-methyl-6,8-diphenyl- (9CI) (CA INDEX NAME)

RN 81153-38-0 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1,8-dimethyl-6-phenyl- (9CI) (CA INDEX NAME)

RN 81153-39-1 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1-methyl-6-phenyl-(9CI) (CA INDEX NAME)

RN 81153-41-5 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-8-methyl-1,6-diphenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1978:517633 CAPLUS

DN 89:117633

TI Hydrolysis and subsequent cyclization of etazolate hydrochloride and related compounds in aqueous solutions: application of PMR and mass spectrometry in accelerated stability studies

AU Puar, Mohindar S.; Funke, Phillip T.; Cohen, Allen I.

CS Squibb Inst. Med. Res., Princeton, NJ, USA

SO Journal of Pharmaceutical Sciences (1978), 67(6), 850-3 CODEN: JPMSAE; ISSN: 0022-3549

DT Journal

LA English

GI

The hydrolysis of etazolate-HCl (I) [35838-58-5], an inhibitor of cyclic nucleotide 3',5'-monophosphate phosphodiesterase that degrades cyclic adenosine 3',5'-monophosphate (cyclic AMP) to AMP, and related compds. was studied by PMR and mass spectrometry. The compds. underwent reversible acid-catalyzed hydrolysis in aqueous solns. at 60°, followed by cyclization to a major and a minor product formed by independent pathways. Under the exptl. conditions, the minor product was stable. The formation rate of the major product 6-ethyl-1,6-dihydrodipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)ione (II) [37649-55-1], was considerably greater than that of the minor component, 3-ethoxy-6-ethyl-1,6-dihydrodipyrazolo[3,4-b:3',4'-d]pyridine (III) [51700-83-5]. For the 6-Me analog (IV) [67324-49-6] of etazolate, the rate of Me deuteration was considerably slower than the rate of cyclization.

RL: BIOL (Biological study)

(etazolate hydrolysis-cyclization product)

RN 37649-55-1 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro- (9CI) (CA INDEX NAME)

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67324-47-4
     RL: BIOL (Biological study)
        (methyletazolate hydrolysis-cyclization product)
RN
     67324-47-4 CAPLUS
    Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-4-methyl-
CN
     (9CI) (CA INDEX NAME)
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ANSWER 8 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     1974:108514 CAPLUS
DN
      80:108514
     Dipyrazolo[3,4-b:3'4'-d]pyridine derivatives and their salts
TI
ΙN
     Hoehn, Hans; Denzel, Theodor
PA
     Chemische Fabrik von Heyden G.m.b.H.
SO
     Ger. Offen., 37 pp.
     CODEN: GWXXBX
DT
     Patent
LΑ
     German
FAN.CNT 1
     PATENT NO.
                        KIND DATE
                                               APPLICATION NO. DATE
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                                               -----
     DE 2333603
                              19740131
                         A1
                                               DE 1973-2333603 19730702
     US 3787430
                         Α
                              19740122
                                               US 1972-271477
                                                                  19720713
     FR 2192831
                        A1
                              19740215
                                               FR 1973-25831
                                                                  19730713
     JP 49051300
                        A2
                              19740518
                                               JP 1973-79725
                                                                  19730713
PRAI US 1972-271477
                              19720713
     For diagram(s), see printed CA Issue.
     Tranquilizing and antiasthmatic dipyrazolopyridines I (R = H, Me, Et,
     CH2Ph, CH2CH2CHMe2, (CH2)3NMe2, COC6H4Cl-p; R1 = Ph, Me, NH2, OEt, OMe, OH, OCH2CHMe2; R2 = Et, CH2Ph) were prepared Thus, 5-amino-1-ethylpyrazole was cyclized with EtoCH:C(COPh)CO2Et to give
     5-benzoyl-1-ethyl-4-hydroxy-1H-pyrazolo[3,4-b]pyridine, which was
     chlorinated and cyclized with N2H4 to I (R = H, R1 = Ph, R2 = Et).
     Treatment with C1(CH2)3NMe2 gave I (R = (CH2)3NMe2, R1 = Ph, R2 = Et).
     37649-62-0P 51700-79-9P 51700-81-3P
     51700-84-6P 51700-85-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
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RN

(Reactant or reagent)

(preparation and alkylation of)

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51700-79-9 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-,
monopotassium salt (9CI) (CA INDEX NAME)
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• I

RN 51700-81-3 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1-(2-furanylmethyl)-1,6-dihydro- (9CI) (CA INDEX NAME)

RN 51700-84-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-4,8-dimethyl- (9CI) (CA INDEX NAME)

RN 51700-85-7 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-4,8-dimethyl-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{N} \\ \hline \\ \text{HN} & \text{N} \\ \hline \\ \text{O} & \text{N} \end{array}$$

RN 51700-88-0 CAPLUS Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-1-(3-methylbutyl)- (9CI) (CA INDEX NAME)

RN 51700-90-4 CAPLUS Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-1-CN (phenylmethyl) - (9CI) (CA INDEX NAME)

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ANSWER 9 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
L4
AN
     1972:514401 CAPLUS
DN
     77:114401
     1,6-Dihydrodipyrazolo[3,4-b:3',4'-d]pyridine-3(2H)-ones
TI
IN
     Hoehn, Hans; Schulze, Ernst
PA
     Chemische Fabrik von Heyden G.m.b.H.
SO
     Ger. Offen., 21 pp.
     CODEN: GWXXBX
DT
     Patent
LΑ
     German
FAN.CNT 2
    PATENT NO.
                     KIND
                           DATE
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APPLICATION NO. DATE DE 2159600 Α 19720608 DE 1971-2159600 19711201 US 3669950 Α 19720613 US 1970-94179 19701201 PRAI US 1970-94179 19701201

GI

For diagram(s), see printed CA Issue. Seven title compds. (I, R = H, Me, CH2CH2OH, R1 = H, Ph, R2 = Et, CH2Ph) and their HCl salts, sedatives, tranquilizers, anxiolytics, and agents for increasing the cellular concentration of adenosine cyclic 3'5'-phosphate, were prepared Reaction of the 5-aminopyrazoles (II) with EtOCH:C(CO2Et)2 gave the di-Et [(5-pyrazolyl)-aminomethylene]malonates (III), which were cyclized in Ph2O at ≤250° to give the Et 4-hydroxy-1H-pyrazolo[3,4-b]pyridine-5-carboxylates (IV). These reacted either with EtI-K2CO3 to give IV 4-ethoxy analogs or with POCl3 to give IV 4-chloro analogs, either of which reacted with RNHNH2 or H2NNHR1 in EtOH in the presence of ZnCl2 to give the 4-hydrazino analogs, which were cyclized with Na in EtoH at reflux to give I. I (R = Rl = H) were methylated to give I (R = Me, R1 = H).

37649-55-1P 37649-58-4P 37649-61-9P 37649-62-0P 37649-63-1P 37649-64-2P IT 39022-83-8P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 37649-55-1 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro- (9CI) (CA INDEX NAME)

RN 37649-58-4 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 37649-61-9 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-2-phenyl-(9CI) (CA INDEX NAME)

RN 37649-62-0 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-1-methyl(9CI) (CA INDEX NAME)

RN 37649-63-1 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1-methyl-6-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 37649-64-2 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-1-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

RN 39022-83-8 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-,
hydrochloride (9CI) (CA INDEX NAME)

●x HCl

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ANSWER 10 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
      1972:488501 CAPLUS
AN
DN
      77:88501
      Dipyrazolo[3,4-B:3',4'-D]-pyridin-3-ones
TI
IN
      Hoehn, Hans; Schulze, Ernest
PA
     E. R. Squibb and Sons, Inc. U.S., 5 pp.
SO
      CODEN: USXXAM
DT
      Patent
LΑ
      English
FAN.CNT 2
      PATENT NO.
                        KIND DATE
                                               APPLICATION NO. DATE
     US 3669950
                         Α
                               19720613
                                               US 1970-94179
                                                                  19701201
     CA 947766
                         A1
                               19740521
                                               CA 1971-128355
                                                                  19711123
     GB 1374310
                               19741120
                                               GB 1971-55068
                                                                  19711126
     HU 164974
                         P
                               19740528
                                               HU 1971-SU693
                                                                  19711130
     DE 2159600
                         Α
                               19720608
                                               DE 1971-2159600
                                                                  19711201
     FR 2116469
                         Α5
                              19720713
                                               FR 1971-43127
                                                                  19711201
     FR 2116469
                         B1
                               19750418
     CH 540274
                         Α
                               19730928
                                               CH 1971-17467
                                                                  19711201
PRAI US 1970-94179
                               19701201
     For diagram(s), see printed CA Issue.
     Dipyrazolopyridinones (I, R = Et, PhCH2; R1 = H, Me, HOCH2CH2; R2 = H, Ph)
     useful as tranquilizers and for increasing intracellular concentration of cyclic
     AMP were prepared by cyclizing hydrazinopyrazolopyridinecarboxylates (II, R3
     = NHNH2, NHNHPh, NMeNH2, N(CH2CH2OH)NH2). Thus, 1-ethyl-5-aminopyrazole
     was condensed with EtOCH:C(CO2Et)2 to 84% Et 1-ethyl-5-
     pyrazolylaminomethylenemalonate which was cyclized to 92% II (R = Et, R3 =
     OH). O-Ethylation of II (R = Et, R3 = OH) and treatment with NH2NH2.H2O gave II (R = Et, R3 = NHNH2), which (10 g) was cyclized to I (R = Et, R1 =
     R2 = H); yield 8.5 g dihydrochloride.
     37649-55-1P 37649-58-4P 37649-61-9P 37649-62-0P 37649-63-1P 37649-64-2P
TΤ
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
RN
     37649-55-1 CAPLUS
     Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro- (9CI)
CN
     (CA INDEX NAME)
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RN 37649-58-4 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 37649-61-9 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-2-phenyl(9CI) (CA INDEX NAME)

RN 37649-62-0 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-1-methyl-(9CI) (CA INDEX NAME)

RN 37649-63-1 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1-methyl-6-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 37649-64-2 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-1-(2-

hydroxyethyl) - (9CI) (CA INDEX NAME)